DOE Hydrogen Codes and Standards Coordinating Committee
Fuel Purity Specifications Workshop
April 26, 2004

Summary Notes
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May 25, 2004

Neil Rossmeissl, DOE Technology Manager for Hydrogen Safety, Codes and Standards, welcomed the attendees and opened the workshop by providing background information on how an R&D plan for fuel purity would fit into the overall codes and standards R&D planning process.

After introductions by the participants, Jim Ohi of NREL reviewed the agenda and the purpose of the workshop, which were to:

1. gain a better understanding of who is doing what in developing fuel purity guidelines and standards in terms of objectives, definitions, scope, timetable, and participants
2. develop a rough work breakdown structure of the fuel purity issue for the total "fuel cycle" for which purity requirements must be defined, including
    a. levels or tiers required for fuel purity corresponding to each segment of the fuel cycle
    b. criteria to develop technically sound and economically viable guidelines or standards
    c. R&D needed to define the levels of purity appropriate for each level or tier
    d. timetable for the guidelines and standards
    e. rough budget for R&D and guideline/standard development.
    f. cost of analysis to ensure appropriate purity level at each segment of the fuel cycle

The desired outcome was to develop a preliminary outline of an R&D plan for hydrogen fuel purity, including a consensus "mini-template" for hydrogen fuel purity specifications that delineates key areas of effort, lead and supporting organizations for each area, and a preliminary outline for an R&D plan with key tasks, timetables, and budgets. The R&D plan for fuel purity will be incorporated in the Codes and Standards R&D Plan, which the Codes and Standards Tech Team of the FreedomCAR and Fuel Partnership is preparing.

To gain a better understanding of current activities, representatives of key organizations gave brief presentations. The presentations will be posted on the DOE Hydrogen, Fuel Cells and Infrastructure Technologies website: www.eere.doe.gov/hydrogenandfuelcells

Addison Bain, ISO TC197 (Hydrogen Technologies)
Dr. Bain described the specifications included in ISO 24687:1999, "Hydrogen Fuel-Product Specification." The standard is based on specifications found in standards developed by the U.S. military, CGA, California, and Japan. The existing ISO standard defines three types of hydrogen fuels: Type l – Gaseous (Grade A (98.0) for ICE/fuel cell/appliances, Grade B (99.90) for industrial applications, Grade C (99.995) for aircraft/space vehicle applications; Type ll – Liquid; and Type llI – Slush. ISO 14687 was released in March 1999 and includes limits for mercury and sulfur in view of fuel cell use and hydrogen production using H_2S.

In 2003, ISO formed WG 12 to update 14687. To date, Type l, Grade D, has been added for fuel cell vehicles (distinct from grade A), as well as limits for formaldehyde and formic acid in view of possible hydrogen production from biomass. The first formal meeting of WG 12 will be held in Tokyo on June 24-25, 2004, in conjunction with the World Hydrogen Energy Conference. The convener of WG 12 is Yasuo Takagi.

Shogo Watanabe – Japan Automotive Research Institute (JARI)
Mr. Watanabe described testing conducted by JARI on the influence of impurities on the performance of single cells. The objective of JARI's work is to help establish hydrogen fuel quality standards for fuel cell vehicles. JARI evaluated existing standards, namely JIS K0512 and ISO 14687, as well as the impurities found in commercially available hydrogen in Japan. JARI conducted single-cell evaluation tests for fuel impurities in which the cell voltage drop ratio (against a reference fuel of seven-9s hydrogen purity) at 1000 mA/cm^2 was measured. As the repeatability of the test was within 2%, a voltage drop ratio of >2% was judged to be due to impurities. Impurities that caused a voltage drop ratio of 2% or greater were CO (at 5-10 ppm), SO_2 (at 2 ppm,) H_2S (at 1-2 ppm), HCHO (at 10-20 ppm), and HCOOH (at 50-100 ppm).

JARI conducted a second set of evaluations that measured the voltage drop ratio of single cells at 1,000 mA/ cm^2 for 10 hours. Impurities that caused such a drop under these test conditions included those mentioned in the previous paragraph and CH_3OH, CH_3COCH_3, and NH_3. Based on this evaluation, JARI identified tentative allowable limits for a number of impurities. JARI concluded that reconsideration of hydrogen fuel quality standards is necessary and has submitted a New Work Item Proposal (NWIP) to ISO/TC197 to amend ISO 14687.

Kazuo Koseki – Engineering Advancement Association of Japan (ENAA)
Mr. Koseki presented the results of the Japan Hydrogen and Fuel Cell Project (JHFC) in which hydrogen produced by reforming desulfurized gasoline (Yokohama Daikoku Station), naptha (Yokohama Asahi Station), LPG (Senju Station), and methanol (Kawasaki Station) were analyzed for fuel purity. Mr. Koseki compared the results of the analysis to the specifications included in the proposed amendment to ISO 14687 and to the JHFC project specifications. The results showed that hydrogen produced in conventional fossil fuel reforming stations satisfies the specification required by ISO and the JHFC project.

Mr. Koseki identified the cost of analysis as a key issue, as it cost each station about $10,000 to analyze hydrogen purity. The cost of analyzers and other equipment for continuous monitoring of fuel purity is estimated to be $50,000 - $150,000 for each station.

Bill Collins (UTC Fuel Cells) – US Fuel Cell Council (USFCC)
Mr. Collins provided an overview of the work to date of the USFCC's Transportation Working Group on the determination of hydrogen specifications for transportation applications. The focus of the USFCC's effort is on the impact of impurities on the fuel cell stack. This focus needs to be integrated with those of on-board fuel storage and hydrogen production, distribution, storage, and dispensing so that a balance between fuel supply costs and vehicle fuel quality requirements can be met. The overall goal of the USFCC is to be part of a coordinated effort of develop a standard for commercial hydrogen fuel purity by 2010.

Mr. Collins outlined the key activities and a general timetable to develop guidelines and standards for fuel purity. The primary role and responsibilities of the USFCC include developing recommendations for fundamental cell testing (cell design and operating parameters, identifying contaminants, recommending a test protocol and matrix) evaluating test information (mechanisms of adverse effects of impurities, reconciliation of diverse test results, relationships between contaminants and impacts due to long and short-term exposures), and regular reporting and revisions as needed.

Mr. Collins presented examples of inputs for a Test Protocol, such as quality control criteria for repeatable and reproducible results; a Test Matrix, for grouping common data by families, contaminant amount, pressure (total and partial), temperature, interactions between contaminants; and a Test Plan to define requirements, apparatus, and measurements. Funding for prioritized testing requirements needs to be provided by the DOE.

Rick Rocheleau – University of Hawaii
Dr. Rocheleau described the capabilities of Hawaii Fuel Cell Test Facility of the University of Hawaii and proposed that the Facility could serve as one of the laboratories for a collaborative fuel purity testing program as long as the hardware is state-of-the-art and non-proprietary so that the information is both relevant and can be shared. The Facility is fully operational with trained staff and has a broad range of gas testing capabilities, including on-line high resolution gas analysis. Dr. Rocheleau is ready to commit significant funds to the fuel purity effort.

Stella Papasavva (GM) – Society of Automotive Engineers
Dr. Papasavva provided an overview of the roles and responsibilities of the SAE Hydrogen Specification Task Force. The objective of the Task Force is to develop an evolving hydrogen fuel purity guideline for the vehicle refueling interface that will mature as the technology advances toward commercial feasibility. This guideline could form the basis for a proposed standard by 2010.

The Task Force is gathering inputs from fuel cell system integrators, on-board storage manufacturers, and fuel providers on allowable fuel purities. Based on these inputs, the Task Force will develop and implement a plan showing how and when different organizations should address key issues. Dr. Papasavva stated that the DOE FreedomCAR and Fuel Partnership and the DOE National laboratories have a leading role in this effort.

Roger Smith – Compressed Gas Association
Mr. Smith described the membership and the standards committees of the Compressed Gas Association. The CGA has 150 members, including industrial gas companies and equipment manufacturers and distributors. There are five CGA committees - Hydrogen Fuel Technology, Bulk Distribution Equipment, Hazardous Materials Codes, Gas Specifications, and Cylinders, Valves and Pressure Relief Devices – that develop standards. The Gas Specifications Committee is developing a draft hydrogen purity standard for stationary fuel cells and ICEs under a DOE/NREL contract. The Committee will use CGA G-5.3 – 2004, "Commodity Specification for Hydrogen," as a starting point. CGA G-5.3-2004 includes specifications for gaseous and liquid hydrogen for typical uses by grade, general sampling methods, general analytical procedures for impurities, and provides a basis for further refinements by suppliers and users.

Questions and comments arose concerning the10-month time frame for the draft standard when fuel cells are yet to be commercialized and more R&D is needed to obtain the numbers that are to be included as specifications in the standard. The CGA and NREL will discuss the timetable in the contract, given the presentations and discussion in the workshop. The CGA will work with other organizations involved, such as the USFCC, and will participate in a subordinate role or lead role to provide expertise to the process. There will most likely be separate standards for stationary and transportation applications, depending on how liability issues emerge with different applications of hydrogen fuel, the use of odorants, and the different value that specialty gases have in the market.

Tony Estrada (PG&E) – American Society of Testing and Materials
Mr. Estrada provided an overview of the ASTM, which has 30,000 members and 20 technical committees, and more detailed information on Committee D03 on Gaseous Fuels. The Committee was formed in 1935 and plays a preeminent role in defining and specifying the methods of sampling, analysis, and testing used in the gaseous fuel industry. The Committee will support the efforts of DOE and other SDOs involved in addressing hydrogen purity specifications by providing information on the physical and chemical characteristics of hydrogen and pertinent test methods for evaluating fuel purity over the full hydrogen fuel cycle. Mr. Estrada described the key activities, work breakdown structures, and budgetary requirements for the Committee to address fuel purity.

Jesse Schneider (Daimler-Chrysler) – California Fuel Cell Partnership
Mr. Schneider chairs the CaFCP's Interoperability and Fuel Purity Group, which is made up of automotive OEMs and fuel providers. The approach of the Group is to develop internal (to the CaFCP) guidelines for interoperability while maintaining active communication with the relevant SDO's. The guidelines are to be used in the pre-commercial phase to help members of the Partnership identify the contaminants that are detrimental to fuel cell systems, the sources of contaminants from different production and delivery pathways, test methods, costs, and lessons learned from demonstration projects. Lessons learned about fuel purity from the demonstrations projects will be brought to the attention of the relevant SDOs.

Walt Podolski (Argonne National Laboratory) – FreedomCAR and Fuel Partnership, Fuel Cell Tech Team
Dr. Podolski gave an overview of the FreedomCAR and Fuel Partnership, which has created 11 technical teams to support the 2015 commercialization decision on hydrogen fuel cell vehicles. The plan of action for each Tech Team is to develop an R&D roadmap and support technology development efforts in defined areas. Six of the eleven Tech Teams are dealing with hydrogen purity: Fuel Cells, Hydrogen Storage, Hydrogen Production, Hydrogen Delivery, Fuel Pathway and Integration, and Codes and Standards.

The Fuel Cell Tech Team wants to avoid premature standards, codes, and regulations that may slow the introduction of new technologies as well as competing national and international SDOs and professional organizations. In turn, the Tech Team encourages flexible guidelines that enable demonstration and validation projects and consistent standards that enable global introduction of fuel cell vehicles. The Tech Team has developed initial specifications for hydrogen purity from the on-board storage system to the fuel cell inlet, and revisions to these specifications are under consideration based on durability data and experience in fuel cell validation projects. The Tech Team is also developing a matrix of impurities and effects.

Brad Smith (Shell Hydrogen)– FreedomCAR and Fuel Partnership, Codes and Standards Tech Team
Mr. Smith discussed the process the Codes and Standards Tech Team is using to develop a Codes and Standards R&D Roadmap. The focus areas of the Roadmap are hydrogen fuel infrastructure, fuel cell vehicles, infrastructure/vehicle interface, and fundamental hydrogen properties. The R&D needs that the Tech Team has identified in addressing fuel purity include resolving data deficits, such as the impact of impurities and diluents on fuel cells; assessing validation and testing possibilities; and assessing the utility and scope of potential interim, pre-commercial guidelines.

The Tech Team will continue R&D within the C&S Roadmap to evolve guidelines to a commercial application. The R&D will be coordinated with the other Tech Teams, including those for Fuel Cells, Production, and Delivery, to establish fuel purity criteria. The Tech Team will also engage industry, academia, and standards and model code development organizations. The potential timeline for establishing these criteria include a Draft Technical Roadmap, identification of early participants, such as national labs and universities), and design of a test protocol and experiments test in 2004; implementation and oversight of experimental test protocol in 2005; a workshop to evaluate results and select guidelines and an assessment of the experience from programs in 2006; and dissemination of information and analysis to standards development organizations in 2007.

After the presentations, Jim Ohi proposed an approach to key issues that need to be resolved to develop a consensus on fuel purity guidelines and specifications. The first step was to sharpen problem definition by identifying key interfaces in the fuel cycle from hydrogen production to hydrogen utilization at the cell level and then compressing the elements of the fuel cycle into three major subgroups: Production/Delivery, Bulk Storage/On-board Storage/Dispensing Systems, and Cell/Stack/Balance of Systems. These three subgroups can serve as the focus areas for teams to address fuel purity issues. As a first step in designating potential lead and supporting organizations in addressing fuel purity over the fuel cycle, Jim identified federal agencies, national laboratories, universities, existing industry-government partnerships, and SDOs involved in each focus area.

Jim then proposed that the problem be approached in four phases that was discussed and amended by the participants.

Phase 0

- Problem definition and disaggregation
- Terminology
- Team building and coordination, especially at the interface of different teams

Phase 1

- Test protocols (vehicle and fuel systems; on-board storage)
- Modeling capabilities, especially degradation mechanisms-linked with advanced diagnostic techniques
- Test Plan, including accelerated testing
- R&D Plan for testing and targets to assess
    - effects of impurities on current state-of-art stacks and fuel systems
    - sources of impurities and detection
    - clean-up options

Phase 2

- Testing
- Data analysis

Phase 3

- Data integration
    - performance, durability, cost
- Preliminary guidelines
- Feedback to Phase 1 and technology development
    - improve tolerance of components to impurities
    - improve capabilities to clean-up on board

        - improve capabilities to reduce impurities in fuels
    - Output to SDOs

To conclude the presentation that was intended to establish a framework for further discussion, Jim proposed that small teams be formed to address each Phase, with the Phase 0 team providing overall coordination of the effort. The Phase 0 team would focus on technical requirements for R&D and analysis; provide a locus for technical coordination and integration of the R&D Planning Team and the Test Teams; and provide outputs to industry-government partnerships, SDOs, and other interested parties.

Discussion of Issues and Needs

Rather than a verbatim summary of the discussion, this summary is organized by issue areas. Also included are insights gained from discussions that Jim Ohi had after the workshop with individual participants.

<u>1. Fuel purity is a misnomer--call it fuel quality (with a minimum purity level implicit)</u>

Fuel purity is a misnomer because it is not purity that is sought as much as the maximum levels of impurities that can be tolerated and yet maintain acceptable performance, durability, and cost of fuel cell systems. The participants agreed to refer to our work as fuel quality rather than fuel purity. In addition, we need to define common terminology for our work products as various groups are developing test protocols, test plans, matrices of impurities, R&D plans, etc.

<u>2. Guidelines based on requirements for evolving, commercially non-viable technology</u>

This discussion focused initially on the potential disconnect of determining the effects of fuel quality on fuel cell stacks that are not commercially viable and that will likely be very different from the current state-of-art when they reach commercial viability; million-dollar cars cannot serve as test beds for fuel quality requirements. At the same time, if one does not know what stack requirements are for fuel quality, how can whole system or upstream fuel infrastructure requirements be realistically addressed? An initial step may be to identify those components and subsystems that may be least likely to change and those for which changes are essential if the technology is to be commercially viable.

While it is important to avoid premature standards, codes, and regulations that may slow the introduction of new technologies, there are important questions concerning the effects of hydrogen fuel quality on the performance and, especially, the durability of fuel cell stacks that need to be addressed. In any case, most of the testing will be done in laboratories, and initial focus of work should be on cells or stacks and on the identification of "bad actors," the key contaminants, and the level of tolerance of cells to each contaminant. Impurities that may have similar characteristics or effects could be grouped, and targets set for each such group of impurities. The aim of this initial work should be to determine what is the "worst" fuel quality that can be used in order to develop minimum guidelines using current state-of-art as a baseline. This initial baseline will provide a starting point and could be based on existing CGA and ISO standards. The baseline should consider the history of gaseous and liquid hydrogen quality, for example, that fuel providers are meeting requirements in CGA 5.3.

Another key initial step will be to classify impurities according to risk—perhaps high, medium, and low—in terms of probability of occurrence (presence in gas stream) and severity of impact on cell and stack performance and durability. We could, in other words, address fuel quality as a risk management problem. Such an approach could serve as a model to approach other R&D issues. An attempt should be made to develop a matrix of impurities by species and key characteristics (especially accumulating vs. self-cleaning impurities) analytic techniques, and sensitivities (to both measurement protocols and cell and stack performance and durability).

Other important issues discussed included the need for low-cost analytical equipment and procedures, and the need to address cathode-side impurities, particularly the effects of impurities in air on cell and stack performance and durability. It was also pointed out that storage materials used in commercially viable systems will also be different from the current state-of-art and that understanding what can storage systems tolerate is important question.

Finally, the work on developing fuel quality guidelines should also allow us to obtain R&D insights and opportunities to better understand key issues and should be much more than a testing program.

3. Understanding mechanisms of degradation due to fuel impurities

The mechanisms of degradation of cell components and materials by impurities and the synergies of the effects of degradation must be better understood. For example, test data cannot be scaled without a better understanding of these mechanisms. There is a critical need to develop cell and stack modeling capabilities to analyze the effects of impurities.
Testing and analysis of breakdown mechanisms, including photomicrograph evidence of degradation, are needed.

4. Cost analysis

It was pointed out that cost analysis of current technology not interesting in that we need to set and address targets because fuel cell stacks will have to change to be competitive. The same point applies to fuel production, distribution, storage, and distribution. A systems analysis approach is needed for total hydrogen system from the fuel cell to production), such as that to be undertaken by the Office of the Systems Integrator for the DOE Hydrogen Program. Also, a major sensitivity analysis is needed to consider what are the elements that drove us toward a particular solution or set of solutions. We need to balance the cost of fuel quality certification needs and the benefits such certification will have on system performance, durability, and cost. To do this, we must work both ends of the problem at the same time and explore hydrogen production processes in terms of the cost in dollars to attain a given fuel quality level.

5. Data compilation, archiving, and distribution

There is no central repository for the data acquired to date, and there is a need for an organization to serve as the library for all of the information needed and that is to be gathered. There is also an issue concerning proprietary data and how the use of non-proprietary data acquired through government-funded R&D and potentially proprietary data acquired through privately funded R&D can be coordinated to advance our knowledge on fuel quality issues.

There is also a need for a centralized and coordinated process to report information. In addition, there should be a coordinated survey to find out what R&D will be helpful to fuel cell manufacturers and other key stakeholders in fuel quality. It would be helpful to have points of contact identified for all of organizations involved in this collaborative effort to address fuel quality.

Next Steps

The overall objectives of the follow-on work will be to identify key impurities, attain a better understanding of the mechanisms of failure due to fuel impurities, and to develop initial guidelines for hydrogen fuel quality to enhance fuel cell efficiency, durability, and market competitiveness. There was discussion that this work should be left to the Office of the Systems Integrator or to the appropriate Tech Teams of the FreedomCAR and Fuel Partnership. The R&D plan for fuel quality, beginning with Phase 0 described earlier, will be a key part of the R&D Roadmap of the Codes and Standards Tech Team and may serve as a model of how other parts of the Roadmap are developed. After the R&D plan for fuel quality is incorporated into the Codes and Standards R&D Roadmap, it will provide guidance for future DOE funding and for solicitations that may be issued for targeted R&D on fuel quality.

Key next steps will be to build on the cooperation that was evident in the workshop. The DOE and NREL will convene a small planning group during the DOE Merit Review meeting in Philadelphia the week of May 24 to develop an overall outline for a Hydrogen Fuel Quality R&D Plan that includes technical and organizational structure, timetable, and budget estimates. This outline will be circulated for review by all of the participants in the workshop. After review, the outline will be fashioned into a more detailed plan that will be incorporated into the overall Codes and Standards R&D Roadmap being developed by the Codes and Standards Tech Team of the FreedomCAR and Fuel Partnership.

Acknowledgments

I would like to thank all of the participants in the workshop, especially those who gave presentations on their activities. I would also like to thank Kristen Rannels of Sentech, Inc., who provided workshop notes and Lara Neer and Brian Schorr of the NHA who made arrangements for the meeting room and equipment.